



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 12:26 am GMT

PDB ID : 6ZXD
EMDB ID : EMD-11517
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State F1
Authors : Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.;
Kutay, U.; Beckmann, R.
Deposited on : 2020-07-29
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

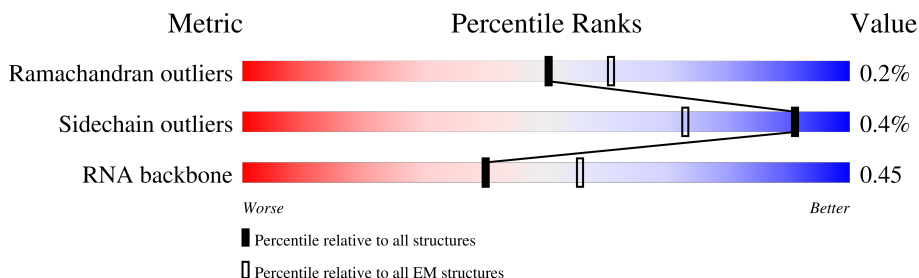
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1873	
2	R	135	
3	A	295	
4	B	264	
5	C	293	
6	E	263	
7	G	249	
8	H	194	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	208	6% 98%
10	J	194	92% 7%
11	L	158	7% 95%
12	N	151	99%
13	O	151	5% 89% 11%
14	V	83	98%
15	W	130	98%
16	X	143	97%
17	Y	133	92% 7%
18	b	84	98%
19	e	59	80% 20%
20	x	252	71% 29%
21	y	412	16% 78% 21%
22	d	56	93% 5%
23	D	243	14% 91% 7%
24	F	204	11% 90% 7%
25	K	165	13% 58% 42%
26	M	132	21% 79% 90% 10%
27	P	145	21% 83% 17%
28	Q	146	94% 5%
29	S	152	27% 94% 6%
30	T	145	10% 99%
31	U	119	23% 85% 15%
32	Z	125	38% 58% 42%
33	c	69	20% 88% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	156	
35	g	317	
36	z	568	
37	k	583	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 80922 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1645	35125	15677	6304	11499	1645	0	0

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	122	990	621	184	182	3	0	0

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	216	1705	1083	299	315	8	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	213	1729	1098	309	308	14	0	0

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	218	1690	1094	289	297	10	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	262	2076	1324	386	358	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	230	1862	1164	371	320	7	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	186	1501	957	276	267	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	205	1682	1056	331	290	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	180	1499	955	300	242	2	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	151	1229	782	230	211	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	149	1202	770	228	203	1	0	0

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	135	1009	618	198	187	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 15 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	47	Total	C	N	O	S	0	0
			375	228	84	62	1		

- Molecule 20 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	x	178	Total	C	N	O	S	0	0
			1391	891	252	244	4		

- Molecule 21 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	y	325	2568	1622	473	463	10	0	0

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	d	55	459	286	94	74	5	0	0

- Molecule 23 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	D	225	1752	1117	315	313	7	0	0

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	F	189	1495	934	284	270	7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	K	95	800	522	142	131	5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	M	119	588	350	119	119	0	0

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	P	120	984	625	184	168	7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 29 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 30 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	f	70	Total	C	N	O	0	0
			346	206	70	70		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	314	2440	1537	425	466	12	0	0

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO1.

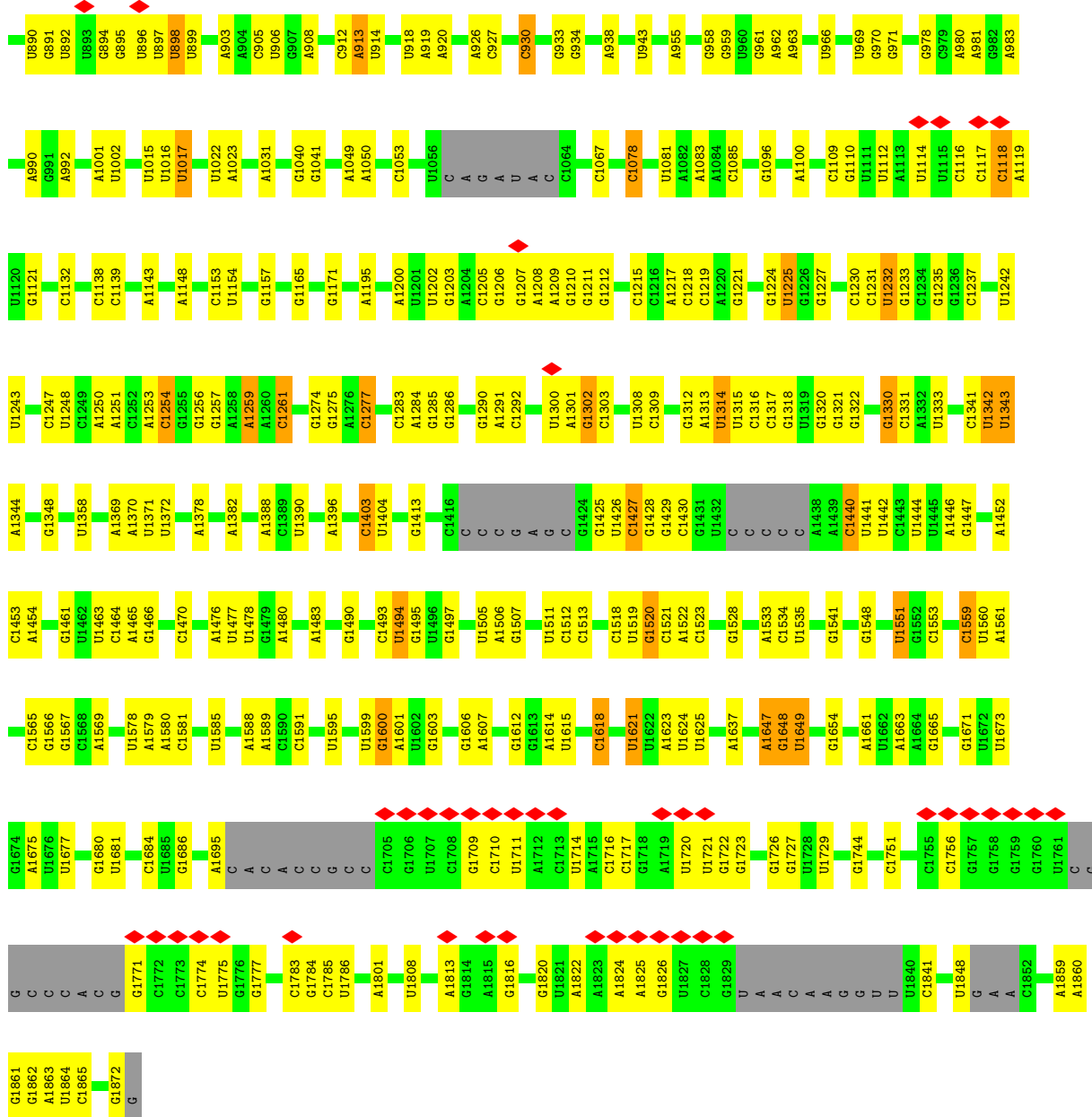
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	z	292	1921	1186	372	353	10	0	0

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

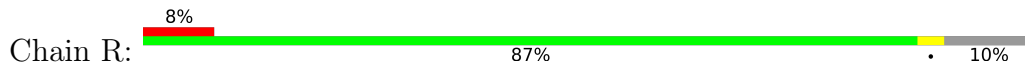
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	k	430	2820	1743	543	527	7	0	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

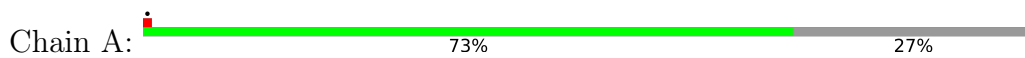
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	2	1	1	1	0
38	y	1	1	1	0

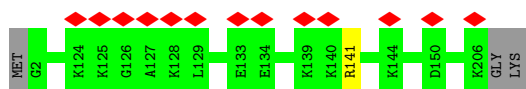


• Molecule 2: 40S ribosomal protein S17

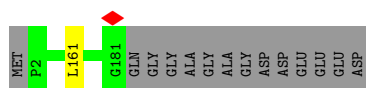


• Molecule 3: 40S ribosomal protein SA

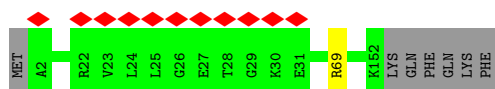




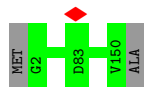
- Molecule 10: 40S ribosomal protein S9



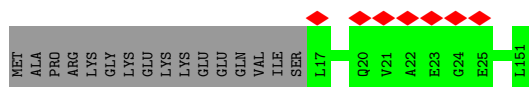
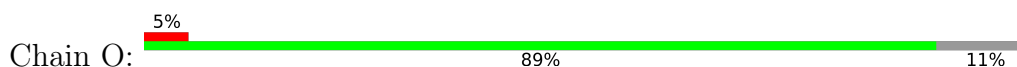
- Molecule 11: 40S ribosomal protein S11



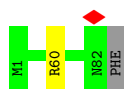
- Molecule 12: 40S ribosomal protein S13



- Molecule 13: 40S ribosomal protein S14



- Molecule 14: 40S ribosomal protein S21



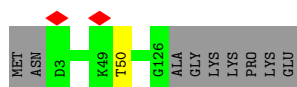
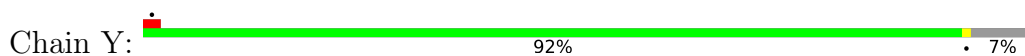
- Molecule 15: 40S ribosomal protein S15a



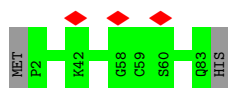
• Molecule 16: 40S ribosomal protein S23



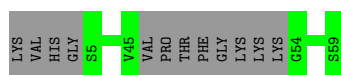
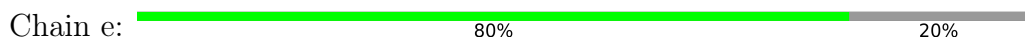
• Molecule 17: 40S ribosomal protein S24



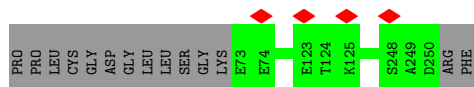
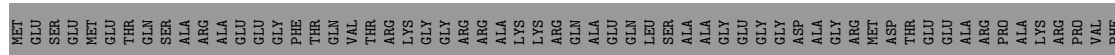
• Molecule 18: 40S ribosomal protein S27



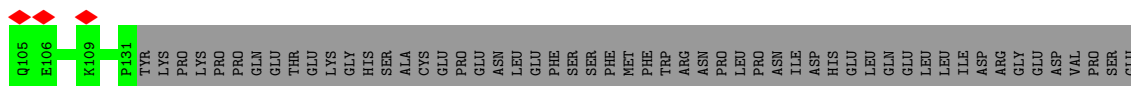
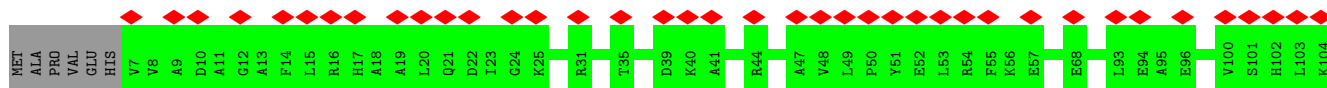
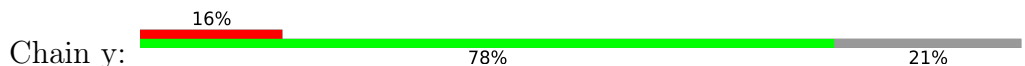
• Molecule 19: 40S ribosomal protein S30

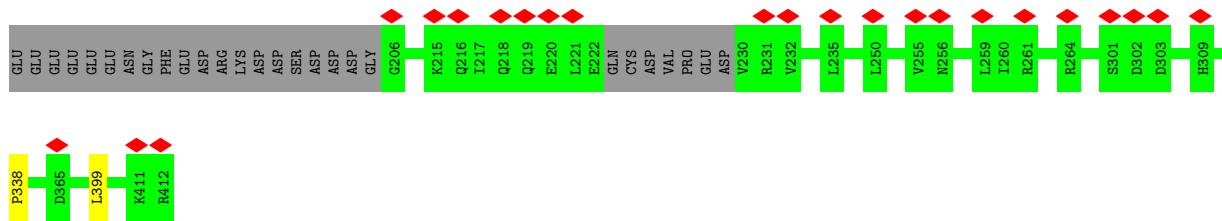


• Molecule 20: RNA-binding protein PNO1



• Molecule 21: RNA-binding protein NOB1

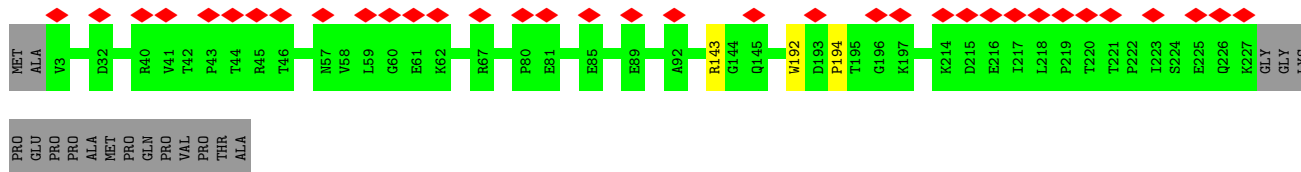
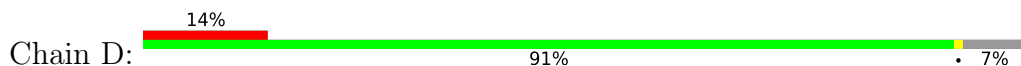




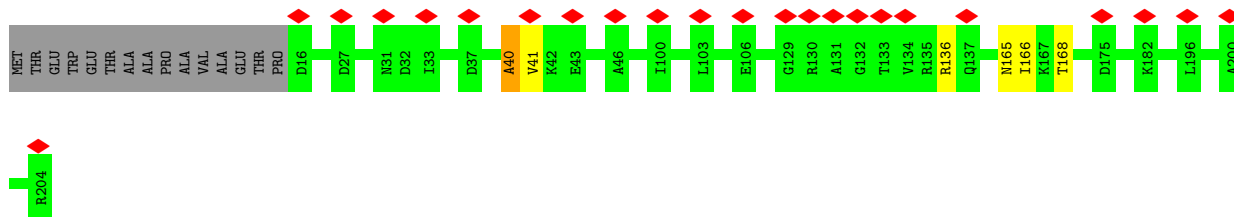
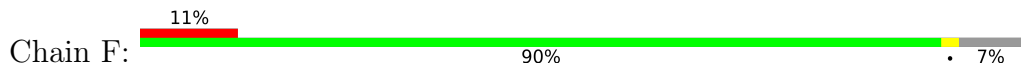
• Molecule 22: 40S ribosomal protein S29



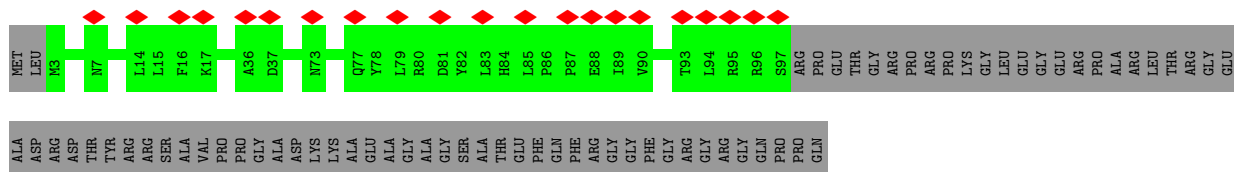
• Molecule 23: 40S ribosomal protein S3



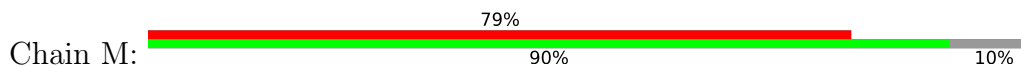
• Molecule 24: 40S ribosomal protein S5

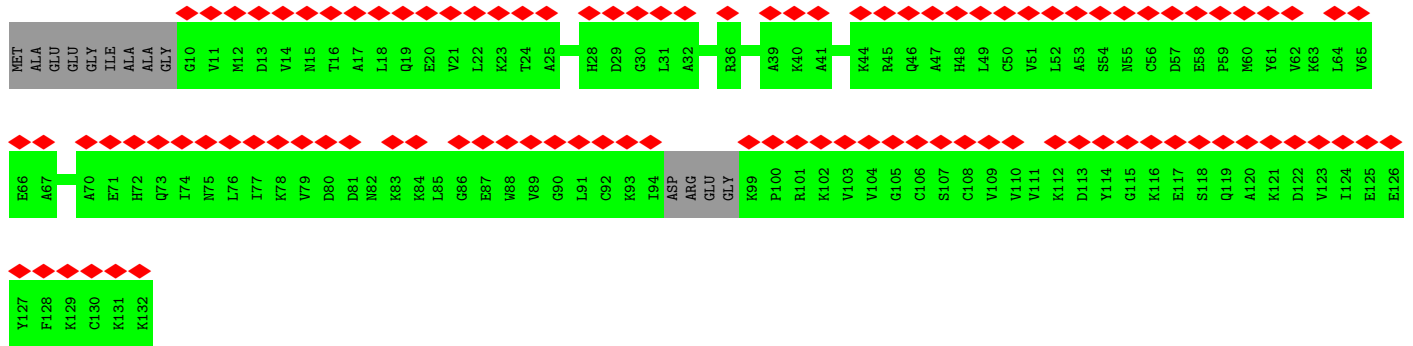


• Molecule 25: 40S ribosomal protein S10

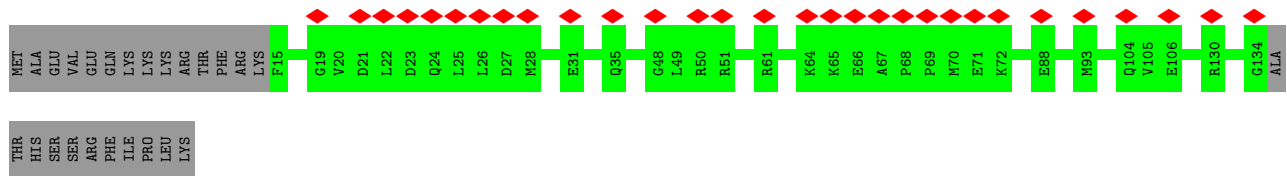
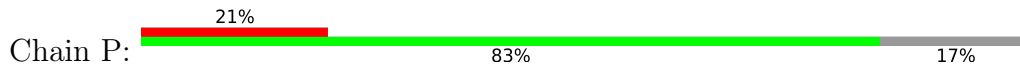


• Molecule 26: 40S ribosomal protein S12

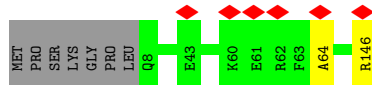




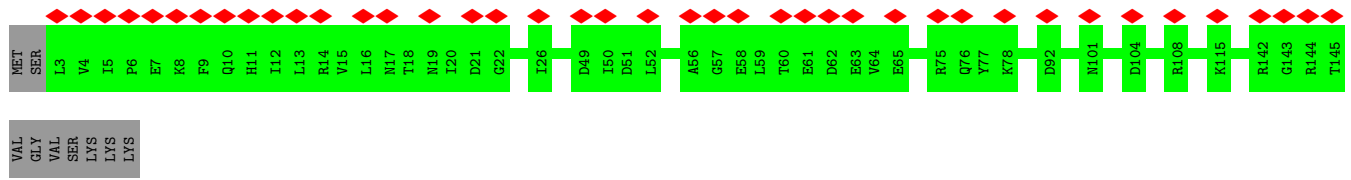
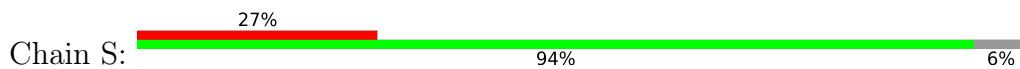
• Molecule 27: 40S ribosomal protein S15



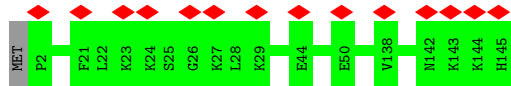
• Molecule 28: 40S ribosomal protein S16



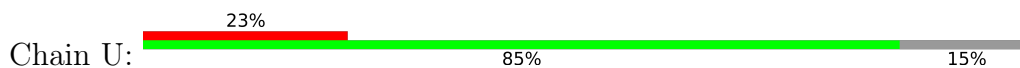
• Molecule 29: 40S ribosomal protein S18

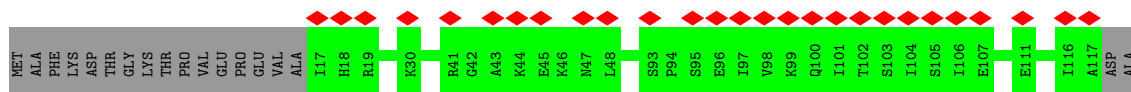


• Molecule 30: 40S ribosomal protein S19

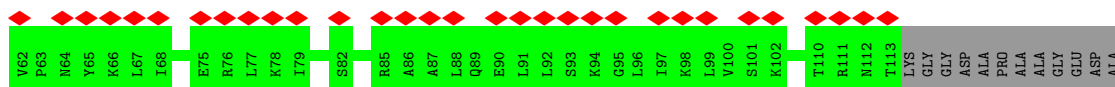
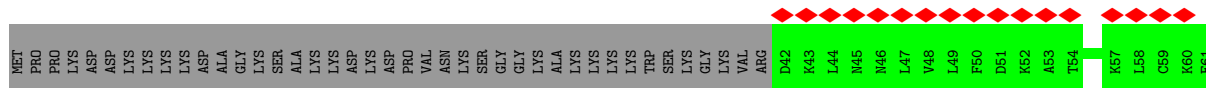


• Molecule 31: 40S ribosomal protein S20

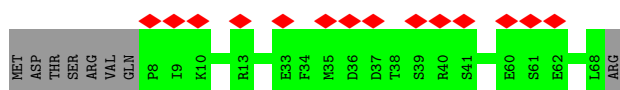
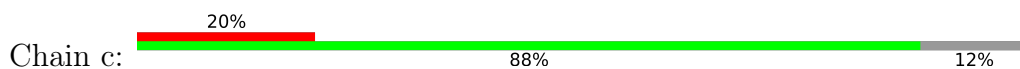




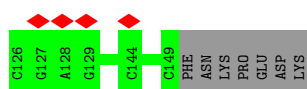
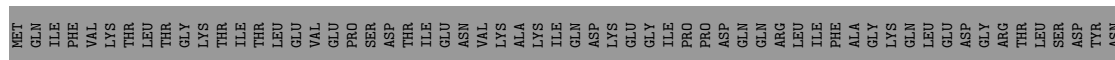
• Molecule 32: 40S ribosomal protein S25



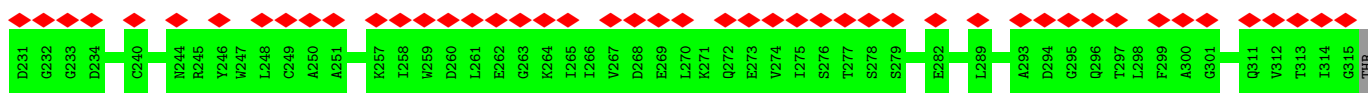
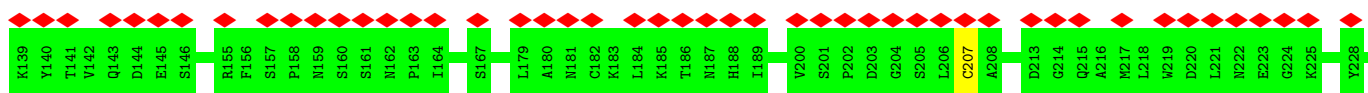
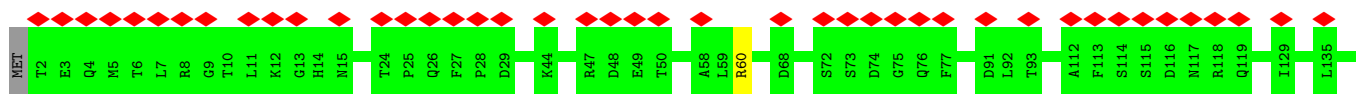
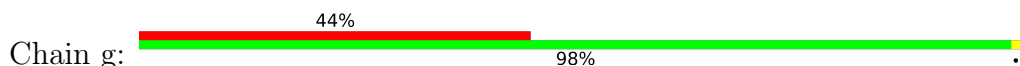
• Molecule 33: 40S ribosomal protein S28



• Molecule 34: Ubiquitin-40S ribosomal protein S27a



• Molecule 35: Receptor of activated protein C kinase 1



I399	V400	P401	L402	G403	R404	K405	E406	A407	K408	A409	K410	E411	Q415	E419	A420	E421	GLU	GLN	R424	S433	G434	Y438	L439	H440	L441	L442	ASP	GLY	N445	E446	N447	Y448	P449	C450	L451	V452	D453	A454	D455	G456	D457	V458	I459	S460	F461	P462	P463	I464	T465	N466	S467	E468	K469	T470	K471							
V472	K473	K474	T475	T476	S477	D478	L479	F480	L481	E482	V483	T484	S485	ALA	THR	S488	L489	Q490	I491	C492	K493	D494	V495	M496	D497	A498	L499	I500	L501	K502	M503	A504	E505	M506	LYS	LYS	TYR	THR	LEU	GLU	ASN	LYS	GLU	GLU	GLY	SER	SER	SER	ASP	THR	THR	GLU	ALA	ALA	ASP	ALA	VAL	VAL	SER	GLY	GLN	LEU
PRO	ASP	PRO	THR	THR	ASN	PRO	SER	ALA	GLY	LYS	ASP	GLY	PRO	SER	LEU	LEU	VAL	VAL	GLN	VAL	ARG	VAL	VAL	VAL	ASP	LEU	GLU	GLY	LEU	LYS	VAL	VAL	VAL	TYR	PRO	SER	LYS	ALA	ASP	LEU	ALA	THR	ALA	PRO	PRO	HIS	VAL	THR	VAL	VAL	VAL	ARG										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.591	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.76	1/39273 (0.0%)	1.10	209/61196 (0.3%)
2	R	0.37	0/1002	0.54	0/1345
3	A	0.43	0/1742	0.56	0/2367
4	B	0.41	0/1756	0.56	1/2350 (0.0%)
5	C	0.46	0/1726	0.57	0/2332
6	E	0.42	0/2118	0.55	1/2849 (0.0%)
7	G	0.37	0/1885	0.52	0/2510
8	H	0.36	0/1524	0.56	0/2042
9	I	0.42	0/1711	0.54	0/2282
10	J	0.44	0/1524	0.56	0/2035
11	L	0.47	0/1250	0.55	0/1673
12	N	0.41	0/1226	0.52	0/1649
13	O	0.37	0/1022	0.56	0/1372
14	V	0.40	0/631	0.54	0/844
15	W	0.48	0/1051	0.57	0/1406
16	X	0.43	0/1116	0.55	0/1490
17	Y	0.43	0/1031	0.56	1/1370 (0.1%)
18	b	0.39	0/653	0.54	0/876
19	e	0.39	0/377	0.52	0/493
20	x	0.41	0/1413	0.59	0/1906
21	y	0.36	0/2618	0.54	1/3536 (0.0%)
22	d	0.40	0/470	0.57	0/623
23	D	0.37	0/1780	0.56	0/2397
24	F	0.32	0/1516	0.53	0/2037
25	K	0.35	0/824	0.58	0/1112
26	M	0.25	0/586	0.49	0/813
27	P	0.36	0/1003	0.51	0/1341
28	Q	0.39	0/1126	0.59	0/1506
29	S	0.32	0/1202	0.53	0/1610
30	T	0.36	0/1142	0.50	0/1530
31	U	0.34	0/813	0.56	0/1092
32	Z	0.30	0/580	0.57	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.32	0/481	0.58	0/643
34	f	0.26	0/344	0.57	0/476
35	g	0.31	0/2497	0.57	0/3399
36	z	0.31	0/1933	0.53	0/2616
37	k	0.29	0/2851	0.57	1/3888 (0.0%)
All	All	0.59	1/85797 (0.0%)	0.87	214/123786 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	R	0	1
16	X	0	1
23	D	0	1
24	F	0	2
37	k	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1254	C	O3'-P	-6.41	1.53	1.61

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	N1-C2-O2	13.98	127.28	118.90
1	2	501	C	C2-N1-C1'	12.30	132.33	118.80
1	2	501	C	N3-C2-O2	-11.76	113.67	121.90
1	2	293	C	N1-C2-O2	11.12	125.57	118.90
1	2	427	U	N3-C2-O2	-9.91	115.26	122.20
1	2	797	C	N1-C2-O2	9.00	124.30	118.90
1	2	293	C	N3-C2-O2	-8.98	115.61	121.90
1	2	659	G	N3-C4-C5	-8.76	124.22	128.60
1	2	1865	C	N1-C2-O2	8.70	124.12	118.90
1	2	1453	C	C2-N1-C1'	8.69	128.36	118.80
1	2	293	C	C2-N1-C1'	8.54	128.20	118.80
1	2	501	C	C6-N1-C2	-8.47	116.91	120.30
1	2	1865	C	N3-C2-O2	-8.44	115.99	121.90
1	2	1453	C	N1-C2-O2	8.40	123.94	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	C6-N1-C1'	-8.39	110.74	120.80
1	2	1016	U	N3-C2-O2	-8.36	116.35	122.20
1	2	1520	G	C4-N9-C1'	8.32	137.31	126.50
1	2	1139	C	C2-N1-C1'	8.29	127.92	118.80
1	2	1618	C	N3-C2-O2	-8.05	116.26	121.90
1	2	1081	U	N3-C2-O2	-8.03	116.58	122.20
1	2	1565	C	C2-N1-C1'	7.97	127.57	118.80
1	2	427	U	N1-C2-O2	7.83	128.28	122.80
1	2	1618	C	N1-C2-O2	7.76	123.55	118.90
1	2	356	C	C2-N1-C1'	7.75	127.33	118.80
1	2	1624	U	N3-C2-O2	-7.70	116.81	122.20
1	2	659	G	C2-N3-C4	7.69	115.75	111.90
1	2	853	C	C6-N1-C2	-7.61	117.25	120.30
1	2	856	C	C2-N1-C1'	7.55	127.11	118.80
1	2	853	C	C2-N1-C1'	7.53	127.09	118.80
1	2	748	C	C5-C6-N1	7.42	124.71	121.00
1	2	797	C	C2-N1-C1'	7.41	126.95	118.80
1	2	356	C	N1-C2-O2	7.40	123.34	118.90
1	2	1139	C	N3-C2-O2	-7.40	116.72	121.90
1	2	1865	C	C2-N1-C1'	7.34	126.88	118.80
1	2	1139	C	N1-C2-O2	7.34	123.30	118.90
1	2	1624	U	C2-N1-C1'	7.27	126.42	117.70
1	2	630	U	C2-N1-C1'	7.26	126.41	117.70
1	2	1016	U	N1-C2-O2	7.23	127.86	122.80
1	2	1520	G	C8-N9-C1'	-7.17	117.68	127.00
37	k	141	LEU	CA-CB-CG	7.16	131.77	115.30
1	2	630	U	N3-C2-O2	-7.15	117.19	122.20
1	2	553	U	C5-C6-N1	7.08	126.24	122.70
1	2	748	C	C2-N1-C1'	7.08	126.59	118.80
1	2	853	C	N3-C2-O2	-7.08	116.95	121.90
1	2	1618	C	C6-N1-C2	-7.04	117.48	120.30
1	2	797	C	N3-C2-O2	-6.98	117.02	121.90
1	2	630	U	N1-C2-O2	6.97	127.68	122.80
1	2	1232	U	C5-C6-N1	6.91	126.16	122.70
1	2	1022	U	C2-N1-C1'	6.89	125.97	117.70
1	2	1403	C	P-O3'-C3'	6.88	127.96	119.70
1	2	356	C	N3-C2-O2	-6.87	117.09	121.90
1	2	427	U	C2-N1-C1'	6.86	125.94	117.70
1	2	1314	U	N3-C2-O2	-6.86	117.40	122.20
1	2	314	U	N3-C2-O2	-6.85	117.41	122.20
1	2	331	C	C2-N1-C1'	6.85	126.33	118.80
1	2	856	C	N1-C2-O2	6.83	123.00	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1551	U	N3-C2-O2	-6.81	117.43	122.20
1	2	1551	U	C2-N1-C1'	6.74	125.79	117.70
1	2	1618	C	C2-N1-C1'	6.71	126.18	118.80
1	2	1302	G	P-O3'-C3'	6.67	127.71	119.70
1	2	853	C	N1-C2-O2	6.66	122.89	118.90
1	2	823	U	N3-C2-O2	-6.60	117.58	122.20
1	2	750	C	C2-N1-C1'	6.60	126.06	118.80
1	2	659	G	N3-C4-N9	6.59	129.96	126.00
17	Y	50	THR	C-N-CA	6.59	138.17	121.70
1	2	1314	U	N1-C2-O2	6.57	127.40	122.80
1	2	659	G	C8-N9-C4	-6.55	103.78	106.40
1	2	553	U	C5-C4-O4	-6.52	121.99	125.90
1	2	1453	C	C5-C6-N1	6.45	124.23	121.00
1	2	1865	C	C6-N1-C2	-6.45	117.72	120.30
1	2	1016	U	C2-N1-C1'	6.36	125.33	117.70
1	2	1494	U	P-O3'-C3'	6.34	127.31	119.70
1	2	1647	A	P-O3'-C3'	6.32	127.29	119.70
1	2	1649	U	N1-C2-O2	6.31	127.22	122.80
1	2	402	C	C5-C6-N1	6.29	124.14	121.00
1	2	1648	G	P-O3'-C3'	6.29	127.24	119.70
1	2	1565	C	N1-C2-O2	6.27	122.67	118.90
1	2	4	C	C6-N1-C2	-6.24	117.80	120.30
1	2	930	C	N1-C2-O2	6.19	122.62	118.90
1	2	547	G	P-O3'-C3'	6.19	127.12	119.70
1	2	1343	U	N1-C2-O2	6.18	127.13	122.80
1	2	114	G	P-O3'-C3'	6.17	127.10	119.70
1	2	1751	C	N1-C2-O2	6.13	122.58	118.90
1	2	1453	C	C6-N1-C2	-6.12	117.85	120.30
1	2	1453	C	N3-C2-O2	-6.11	117.62	121.90
1	2	1551	U	N1-C2-O2	6.10	127.07	122.80
1	2	1078	C	C2-N1-C1'	6.09	125.50	118.80
1	2	334	C	C6-N1-C2	-6.08	117.87	120.30
1	2	1624	U	N1-C2-O2	6.07	127.05	122.80
1	2	1081	U	N1-C2-O2	6.04	127.03	122.80
1	2	293	C	C6-N1-C2	-6.03	117.89	120.30
1	2	1078	C	C6-N1-C2	-6.01	117.89	120.30
1	2	1714	U	N3-C2-O2	-6.01	117.99	122.20
1	2	1015	U	C2-N3-C4	-6.00	123.40	127.00
1	2	1565	C	OP1-P-O3'	6.00	118.41	105.20
1	2	178	C	N1-C2-O2	6.00	122.50	118.90
1	2	143	U	P-O3'-C3'	5.99	126.89	119.70
1	2	1232	U	C6-N1-C2	-5.98	117.41	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1565	C	C5-C6-N1	5.95	123.97	121.00
1	2	632	C	C2-N1-C1'	5.94	125.33	118.80
1	2	1277	C	N1-C2-O2	5.92	122.45	118.90
1	2	1261	C	N1-C2-O2	5.91	122.45	118.90
1	2	1751	C	N3-C2-O2	-5.88	117.78	121.90
1	2	898	U	C2-N1-C1'	5.88	124.76	117.70
1	2	1259	A	C2-N3-C4	5.88	113.54	110.60
1	2	1139	C	C6-N1-C2	-5.86	117.96	120.30
1	2	1453	C	C6-N1-C1'	-5.84	113.79	120.80
1	2	168	C	C2-N1-C1'	5.84	125.22	118.80
1	2	871	U	O5'-P-OP2	5.84	117.70	110.70
1	2	1625	U	C2-N1-C1'	5.84	124.70	117.70
1	2	1017	U	N1-C2-O2	5.82	126.88	122.80
1	2	632	C	C5-C6-N1	5.82	123.91	121.00
1	2	501	C	C5-C6-N1	5.81	123.90	121.00
1	2	151	C	C2-N1-C1'	5.80	125.18	118.80
1	2	441	C	C2-N1-C1'	5.80	125.18	118.80
1	2	926	A	N3-C4-N9	5.79	132.03	127.40
1	2	659	G	C4-N9-C1'	5.79	134.03	126.50
1	2	1520	G	P-O3'-C3'	5.79	126.65	119.70
1	2	593	C	C2-N1-C1'	5.77	125.14	118.80
1	2	1649	U	N3-C2-O2	-5.75	118.17	122.20
1	2	1330	G	P-O3'-C3'	5.75	126.60	119.70
1	2	1684	C	N1-C2-O2	5.75	122.35	118.90
1	2	1440	C	C6-N1-C2	-5.74	118.00	120.30
1	2	293	C	C6-N1-C1'	-5.74	113.92	120.80
1	2	369	C	C2-N1-C1'	5.73	125.10	118.80
1	2	553	U	C2-N1-C1'	5.71	124.56	117.70
1	2	102	A	P-O3'-C3'	5.71	126.55	119.70
1	2	1017	U	N3-C2-O2	-5.71	118.20	122.20
1	2	1717	C	C5-C6-N1	5.70	123.85	121.00
1	2	1139	C	C6-N1-C1'	-5.67	114.00	120.80
1	2	1343	U	N3-C2-O2	-5.66	118.24	122.20
1	2	791	C	P-O3'-C3'	5.65	126.48	119.70
1	2	168	C	N1-C2-O2	5.65	122.29	118.90
1	2	334	C	C2-N1-C1'	5.60	124.96	118.80
1	2	334	C	C5-C6-N1	5.60	123.80	121.00
1	2	553	U	N3-C4-O4	5.60	123.32	119.40
1	2	1118	C	C2-N1-C1'	5.60	124.96	118.80
1	2	1716	C	N3-C2-O2	-5.60	117.98	121.90
1	2	1342	U	P-O3'-C3'	5.60	126.42	119.70
1	2	441	C	C6-N1-C2	-5.60	118.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	898	U	N1-C2-O2	5.59	126.71	122.80
1	2	1625	U	C5-C6-N1	5.59	125.50	122.70
1	2	1565	C	C6-N1-C1'	-5.58	114.10	120.80
1	2	178	C	N3-C2-O2	-5.58	118.00	121.90
1	2	926	A	C4-N9-C1'	5.57	136.32	126.30
1	2	4	C	C2-N1-C1'	5.57	124.92	118.80
1	2	624	C	C6-N1-C2	-5.56	118.08	120.30
1	2	1716	C	N1-C2-O2	5.56	122.24	118.90
1	2	797	C	C6-N1-C1'	-5.55	114.14	120.80
1	2	1565	C	P-O3'-C3'	5.52	126.33	119.70
1	2	856	C	C6-N1-C1'	-5.52	114.18	120.80
1	2	539	C	N1-C2-O2	5.51	122.21	118.90
1	2	427	U	C6-N1-C2	-5.49	117.70	121.00
6	E	38	LEU	CA-CB-CG	5.49	127.93	115.30
1	2	340	C	N1-C2-O2	5.49	122.19	118.90
1	2	1621	U	C2-N1-C1'	5.48	124.28	117.70
1	2	1230	C	C6-N1-C2	-5.47	118.11	120.30
1	2	331	C	C6-N1-C1'	-5.47	114.24	120.80
1	2	748	C	C6-N1-C2	-5.46	118.12	120.30
1	2	1235	G	C4-N9-C1'	5.44	133.57	126.50
1	2	119	U	N3-C2-O2	-5.44	118.39	122.20
1	2	1714	U	N1-C2-O2	5.42	126.59	122.80
1	2	1520	G	N3-C4-N9	5.42	129.25	126.00
1	2	71	G	C4-N9-C1'	5.40	133.52	126.50
1	2	168	C	N3-C2-O2	-5.39	118.13	121.90
1	2	1022	U	N1-C2-O2	5.38	126.57	122.80
1	2	356	C	C6-N1-C1'	-5.38	114.35	120.80
1	2	1600	G	N3-C4-N9	5.38	129.23	126.00
1	2	1684	C	N3-C2-O2	-5.36	118.15	121.90
1	2	624	C	C5-C6-N1	5.36	123.68	121.00
1	2	143	U	OP2-P-O3'	5.34	116.95	105.20
1	2	913	A	O4'-C1'-N9	5.34	112.47	108.20
1	2	666	U	C2-N1-C1'	5.34	124.11	117.70
1	2	1600	G	C4-N9-C1'	5.33	133.44	126.50
1	2	1427	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1565	C	C6-N1-C2	-5.33	118.17	120.30
1	2	824	C	N1-C2-O2	5.32	122.09	118.90
1	2	465	A	P-O3'-C3'	5.31	126.07	119.70
1	2	321	C	C2-N1-C1'	5.30	124.64	118.80
1	2	750	C	C5-C6-N1	5.30	123.65	121.00
1	2	1235	G	C8-N9-C1'	-5.30	120.11	127.00
1	2	1261	C	N3-C2-O2	-5.29	118.20	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	369	C	N1-C2-O2	5.29	122.07	118.90
1	2	632	C	C6-N1-C2	-5.26	118.19	120.30
1	2	1595	U	N1-C2-O2	5.26	126.48	122.80
1	2	811	A	P-O3'-C3'	5.26	126.01	119.70
1	2	1396	A	O4'-C1'-N9	5.24	112.39	108.20
4	B	62	LEU	CA-CB-CG	5.24	127.35	115.30
1	2	809	A	N7-C8-N9	5.23	116.42	113.80
1	2	331	C	N1-C2-O2	5.22	122.03	118.90
1	2	1600	G	N3-C4-C5	-5.21	126.00	128.60
1	2	118	C	N1-C2-O2	5.20	122.02	118.90
1	2	338	G	C4-N9-C1'	5.18	133.23	126.50
1	2	1751	C	C2-N1-C1'	5.18	124.50	118.80
1	2	71	G	N3-C4-C5	-5.17	126.02	128.60
1	2	749	U	P-O3'-C3'	5.17	125.90	119.70
1	2	1684	C	C6-N1-C2	-5.17	118.23	120.30
1	2	402	C	C6-N1-C2	-5.16	118.24	120.30
21	y	399	LEU	C-N-CA	-5.14	108.84	121.70
1	2	1771	G	C4-N9-C1'	5.14	133.18	126.50
1	2	532	C	C2-N1-C1'	5.13	124.45	118.80
1	2	926	A	C8-N9-C1'	-5.13	118.47	127.70
1	2	162	C	C6-N1-C2	-5.13	118.25	120.30
1	2	856	C	C5-C6-N1	5.11	123.56	121.00
1	2	1774	C	N1-C2-O2	5.11	121.97	118.90
1	2	877	C	C6-N1-C2	-5.07	118.27	120.30
1	2	1261	C	C6-N1-C2	-5.04	118.28	120.30
1	2	1591	C	N1-C2-O2	5.04	121.92	118.90
1	2	809	A	C8-N9-C4	-5.03	103.79	105.80
1	2	1225	U	N3-C2-O2	-5.03	118.68	122.20
1	2	180	G	P-O3'-C3'	5.02	125.73	119.70
1	2	1559	C	C5-C6-N1	5.02	123.51	121.00
1	2	750	C	N1-C2-O2	5.01	121.91	118.90
1	2	966	U	N3-C2-O2	-5.01	118.69	122.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	D	194	PRO	Peptide
24	F	165	ASN	Peptide
24	F	40	ALA	Peptide
2	R	74	GLN	Peptide
16	X	60	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
37	k	124	GLU	Peptide
37	k	461	PHE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	120/135 (89%)	109 (91%)	8 (7%)	3 (2%)	5	32
3	A	214/295 (72%)	202 (94%)	12 (6%)	0	100	100
4	B	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
5	C	216/293 (74%)	206 (95%)	10 (5%)	0	100	100
6	E	260/263 (99%)	243 (94%)	17 (6%)	0	100	100
7	G	228/249 (92%)	213 (93%)	15 (7%)	0	100	100
8	H	184/194 (95%)	171 (93%)	13 (7%)	0	100	100
9	I	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
10	J	178/194 (92%)	166 (93%)	11 (6%)	1 (1%)	25	64
11	L	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
12	N	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
13	O	133/151 (88%)	120 (90%)	13 (10%)	0	100	100
14	V	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
15	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
16	X	139/143 (97%)	133 (96%)	5 (4%)	1 (1%)	22	61
17	Y	122/133 (92%)	115 (94%)	7 (6%)	0	100	100
18	b	80/84 (95%)	72 (90%)	8 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	e	43/59 (73%)	41 (95%)	2 (5%)	0	100	100
20	x	176/252 (70%)	168 (96%)	8 (4%)	0	100	100
21	y	319/412 (77%)	288 (90%)	30 (9%)	1 (0%)	41	74
22	d	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	8	39
23	D	223/243 (92%)	210 (94%)	12 (5%)	1 (0%)	34	69
24	F	187/204 (92%)	165 (88%)	19 (10%)	3 (2%)	9	43
25	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
26	M	115/132 (87%)	102 (89%)	13 (11%)	0	100	100
27	P	118/145 (81%)	113 (96%)	5 (4%)	0	100	100
28	Q	137/146 (94%)	123 (90%)	13 (10%)	1 (1%)	22	61
29	S	141/152 (93%)	131 (93%)	10 (7%)	0	100	100
30	T	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
31	U	99/119 (83%)	93 (94%)	6 (6%)	0	100	100
32	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
33	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
34	f	66/156 (42%)	51 (77%)	15 (23%)	0	100	100
35	g	312/317 (98%)	280 (90%)	32 (10%)	0	100	100
36	z	282/568 (50%)	255 (90%)	27 (10%)	0	100	100
37	k	418/583 (72%)	374 (90%)	44 (10%)	0	100	100
All	All	5844/7176 (81%)	5411 (93%)	421 (7%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	F	166	ILE
28	Q	64	ALA
2	R	87	GLU
10	J	161	LEU
21	y	338	PRO
2	R	75	GLU
22	d	13	LYS
23	D	192	TRP
24	F	40	ALA
24	F	41	VAL
16	X	86	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	42	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	110/122 (90%)	110 (100%)	0	100	100
3	A	180/243 (74%)	180 (100%)	0	100	100
4	B	194/231 (84%)	193 (100%)	1 (0%)	88	95
5	C	184/225 (82%)	182 (99%)	2 (1%)	73	88
6	E	224/225 (100%)	224 (100%)	0	100	100
7	G	200/218 (92%)	199 (100%)	1 (0%)	88	95
8	H	167/174 (96%)	167 (100%)	0	100	100
9	I	178/180 (99%)	177 (99%)	1 (1%)	86	94
10	J	160/168 (95%)	160 (100%)	0	100	100
11	L	135/142 (95%)	134 (99%)	1 (1%)	84	94
12	N	130/131 (99%)	130 (100%)	0	100	100
13	O	105/119 (88%)	105 (100%)	0	100	100
14	V	66/67 (98%)	65 (98%)	1 (2%)	65	85
15	W	112/113 (99%)	111 (99%)	1 (1%)	78	91
16	X	113/115 (98%)	112 (99%)	1 (1%)	78	91
17	Y	108/115 (94%)	108 (100%)	0	100	100
18	b	74/76 (97%)	74 (100%)	0	100	100
19	e	38/48 (79%)	38 (100%)	0	100	100
20	x	150/208 (72%)	150 (100%)	0	100	100
21	y	285/367 (78%)	285 (100%)	0	100	100
22	d	48/49 (98%)	46 (96%)	2 (4%)	30	65
23	D	189/202 (94%)	188 (100%)	1 (0%)	88	95
24	F	159/170 (94%)	157 (99%)	2 (1%)	69	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	K	86/136 (63%)	86 (100%)	0	100	100
27	P	107/130 (82%)	107 (100%)	0	100	100
28	Q	115/121 (95%)	114 (99%)	1 (1%)	78	91
29	S	124/132 (94%)	124 (100%)	0	100	100
30	T	114/115 (99%)	114 (100%)	0	100	100
31	U	93/107 (87%)	93 (100%)	0	100	100
32	Z	64/103 (62%)	64 (100%)	0	100	100
33	c	54/62 (87%)	54 (100%)	0	100	100
35	g	272/275 (99%)	270 (99%)	2 (1%)	84	94
36	z	135/512 (26%)	135 (100%)	0	100	100
37	k	215/487 (44%)	212 (99%)	3 (1%)	67	86
All	All	4688/5888 (80%)	4668 (100%)	20 (0%)	91	95

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	88	THR
5	C	68	ARG
5	C	248	TYR
7	G	92	ARG
9	I	141	ARG
11	L	69	ARG
14	V	60	ARG
15	W	104	LEU
16	X	115	ILE
22	d	3	HIS
22	d	5	GLN
23	D	143	ARG
24	F	136	ARG
24	F	168	THR
28	Q	146	ARG
35	g	60	ARG
35	g	207	CYS
37	k	150	ARG
37	k	242	LEU
37	k	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67)

such sidechains are listed below:

Mol	Chain	Res	Type
2	R	29	HIS
2	R	83	ASN
2	R	116	ASN
3	A	84	GLN
3	A	131	HIS
4	B	40	ASN
4	B	53	GLN
4	B	95	ASN
4	B	159	GLN
4	B	186	ASN
6	E	8	HIS
6	E	98	ASN
6	E	179	ASN
6	E	188	ASN
7	G	56	ASN
7	G	81	HIS
8	H	25	GLN
8	H	114	GLN
9	I	84	ASN
9	I	116	HIS
9	I	165	GLN
10	J	125	HIS
11	L	18	GLN
11	L	83	GLN
11	L	112	HIS
12	N	5	HIS
12	N	58	HIS
13	O	113	GLN
15	W	24	GLN
15	W	64	ASN
16	X	46	HIS
18	b	65	GLN
20	x	106	GLN
20	x	232	ASN
21	y	26	ASN
21	y	102	HIS
21	y	348	GLN
21	y	353	GLN
21	y	386	GLN
23	D	101	GLN
24	F	83	ASN
24	F	107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	F	110	GLN
24	F	114	ASN
24	F	179	ASN
24	F	203	ASN
27	P	32	GLN
27	P	41	GLN
27	P	103	ASN
28	Q	11	GLN
28	Q	35	ASN
29	S	134	GLN
30	T	126	GLN
31	U	100	GLN
32	Z	103	HIS
32	Z	112	ASN
35	g	64	HIS
35	g	76	GLN
35	g	119	GLN
35	g	237	ASN
36	z	121	ASN
36	z	548	ASN
37	k	53	HIS
37	k	78	HIS
37	k	139	ASN
37	k	156	GLN
37	k	212	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1632/1873 (87%)	469 (28%)	41 (2%)

All (469) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	11	A
1	2	23	G
1	2	25	A
1	2	33	G
1	2	41	G
1	2	44	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	46	A
1	2	50	A
1	2	56	G
1	2	58	C
1	2	61	A
1	2	62	G
1	2	64	A
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	99	A
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	127	C
1	2	128	U
1	2	129	C
1	2	130	G
1	2	142	C
1	2	143	U
1	2	144	U
1	2	155	G
1	2	157	U
1	2	163	U
1	2	167	G
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	183	G
1	2	184	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	189	U
1	2	190	G
1	2	214	U
1	2	215	G
1	2	290	U
1	2	291	G
1	2	292	A
1	2	295	C
1	2	305	U
1	2	306	C
1	2	310	C
1	2	312	G
1	2	315	C
1	2	319	C
1	2	332	G
1	2	333	G
1	2	334	C
1	2	338	G
1	2	347	G
1	2	353	C
1	2	357	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C
1	2	382	C
1	2	385	G
1	2	386	C
1	2	387	C
1	2	400	C
1	2	408	A
1	2	409	C
1	2	413	G
1	2	418	A
1	2	421	G
1	2	428	U
1	2	429	C
1	2	436	G
1	2	441	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	469	A
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	487	U
1	2	492	C
1	2	493	A
1	2	500	A
1	2	502	C
1	2	516	A
1	2	518	G
1	2	531	A
1	2	532	C
1	2	534	G
1	2	536	A
1	2	541	U
1	2	542	U
1	2	544	G
1	2	545	A
1	2	548	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	594	A
1	2	598	G
1	2	600	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	621	C
1	2	626	G
1	2	628	A
1	2	629	A
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	656	G
1	2	659	G
1	2	660	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	685	A
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	752	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	798	G
1	2	799	U
1	2	809	A
1	2	810	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	812	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	830	A
1	2	834	C
1	2	847	A
1	2	856	C
1	2	861	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	882	U
1	2	885	U
1	2	886	A
1	2	887	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	894	G
1	2	895	G
1	2	896	U
1	2	897	U
1	2	898	U
1	2	899	U
1	2	903	A
1	2	905	C
1	2	906	U
1	2	908	A
1	2	913	A
1	2	914	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	927	C
1	2	930	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	955	A
1	2	959	G
1	2	961	G
1	2	962	A
1	2	963	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	978	G
1	2	981	A
1	2	983	A
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1031	A
1	2	1040	G
1	2	1041	G
1	2	1049	A
1	2	1050	A
1	2	1053	C
1	2	1067	C
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1096	G
1	2	1100	A
1	2	1109	C
1	2	1110	G
1	2	1112	U
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1121	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1132	C
1	2	1138	C
1	2	1143	A
1	2	1148	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1165	G
1	2	1171	G
1	2	1195	A
1	2	1200	A
1	2	1202	U
1	2	1203	G
1	2	1205	C
1	2	1206	G
1	2	1207	G
1	2	1208	A
1	2	1209	A
1	2	1210	G
1	2	1211	G
1	2	1212	G
1	2	1215	C
1	2	1217	A
1	2	1218	C
1	2	1219	C
1	2	1221	G
1	2	1224	G
1	2	1225	U
1	2	1227	G
1	2	1232	U
1	2	1233	G
1	2	1237	C
1	2	1242	U
1	2	1243	U
1	2	1248	U
1	2	1250	A
1	2	1251	A
1	2	1253	A
1	2	1254	C
1	2	1256	G
1	2	1257	G
1	2	1259	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1261	C
1	2	1274	G
1	2	1275	G
1	2	1277	C
1	2	1283	C
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1291	A
1	2	1292	C
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1318	G
1	2	1320	G
1	2	1321	G
1	2	1322	G
1	2	1331	C
1	2	1333	U
1	2	1341	C
1	2	1342	U
1	2	1343	U
1	2	1344	A
1	2	1348	G
1	2	1358	U
1	2	1369	A
1	2	1370	A
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1382	A
1	2	1388	A
1	2	1390	U
1	2	1403	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1404	U
1	2	1413	G
1	2	1425	G
1	2	1426	U
1	2	1427	C
1	2	1428	G
1	2	1429	G
1	2	1430	C
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1447	G
1	2	1452	A
1	2	1454	A
1	2	1461	G
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1470	C
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1480	A
1	2	1483	A
1	2	1490	G
1	2	1493	C
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1512	C
1	2	1513	C
1	2	1518	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1523	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1528	G
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1541	G
1	2	1548	G
1	2	1551	U
1	2	1553	C
1	2	1559	C
1	2	1560	U
1	2	1561	A
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1578	U
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1585	U
1	2	1588	A
1	2	1589	A
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1603	G
1	2	1606	G
1	2	1607	A
1	2	1612	G
1	2	1614	A
1	2	1615	U
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1647	A
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1661	A
1	2	1663	A
1	2	1665	G
1	2	1671	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1673	U
1	2	1675	A
1	2	1677	U
1	2	1680	G
1	2	1681	U
1	2	1686	G
1	2	1695	A
1	2	1709	G
1	2	1710	C
1	2	1711	U
1	2	1720	U
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1775	U
1	2	1777	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1801	A
1	2	1808	U
1	2	1813	A
1	2	1816	G
1	2	1820	G
1	2	1822	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1841	C
1	2	1848	U
1	2	1859	A
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1872	G

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	465	A
1	2	547	G
1	2	604	A
1	2	749	U
1	2	750	C
1	2	791	C
1	2	811	A
1	2	870	A
1	2	912	C
1	2	958	G
1	2	980	A
1	2	1209	A
1	2	1231	C
1	2	1232	U
1	2	1247	C
1	2	1290	G
1	2	1302	G
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1369	A
1	2	1403	C
1	2	1425	G
1	2	1427	C
1	2	1440	C
1	2	1464	C
1	2	1494	U
1	2	1511	U
1	2	1520	G
1	2	1534	C
1	2	1606	G
1	2	1647	A
1	2	1648	G
1	2	1726	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

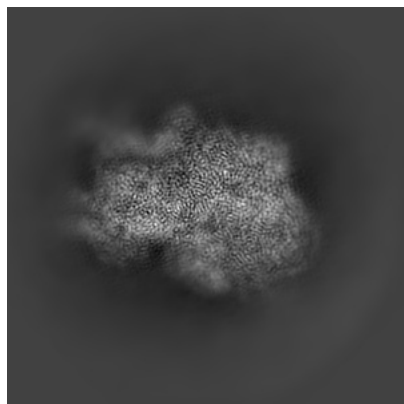
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11517. These allow visual inspection of the internal detail of the map and identification of artifacts.

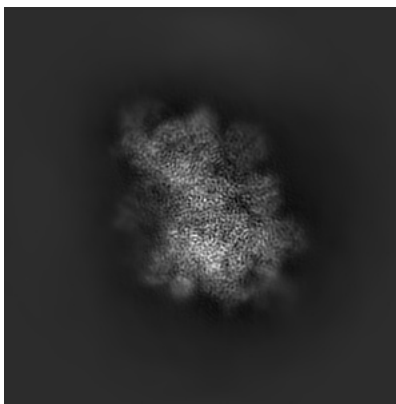
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

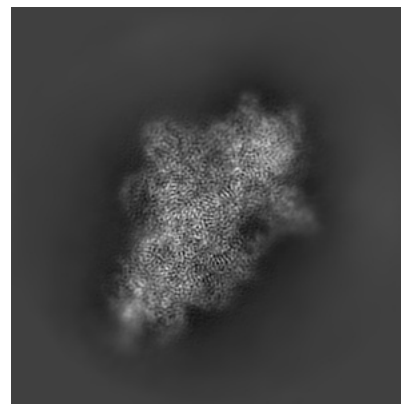
6.1.1 Primary map



X

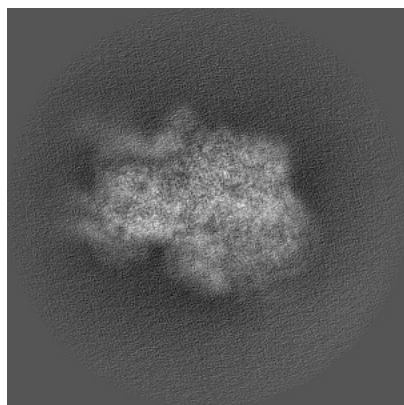


Y

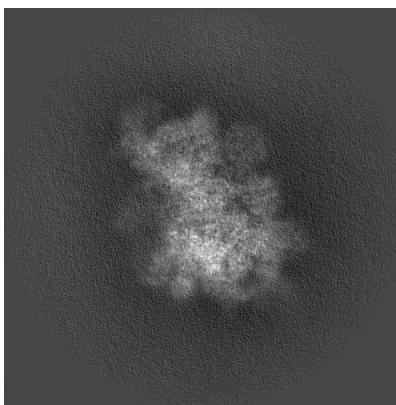


Z

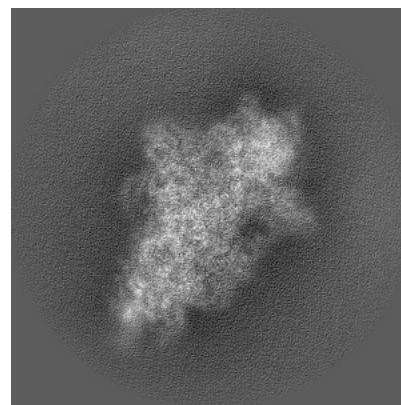
6.1.2 Raw map



X



Y

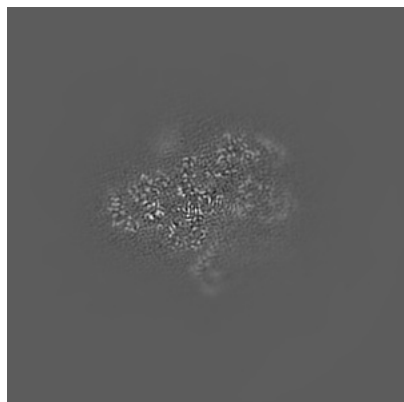


Z

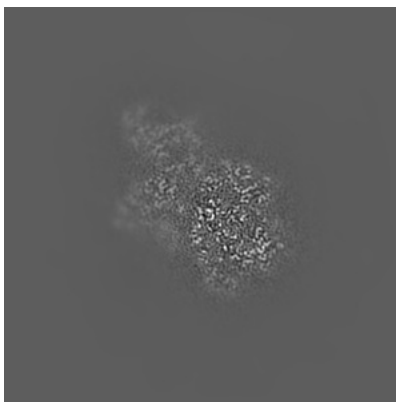
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

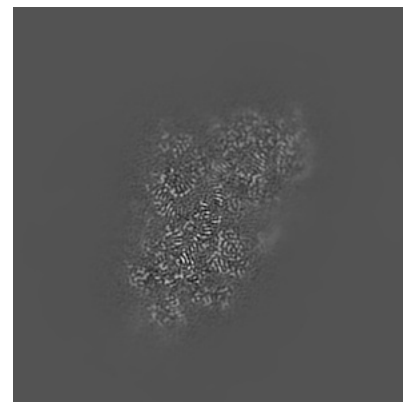
6.2.1 Primary map



X Index: 180

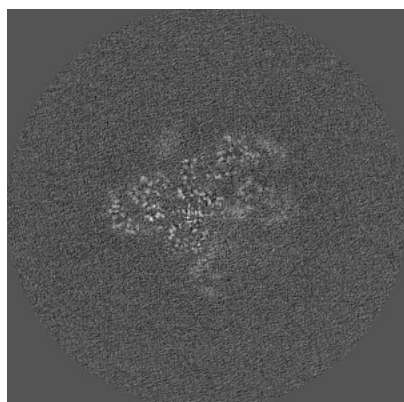


Y Index: 180

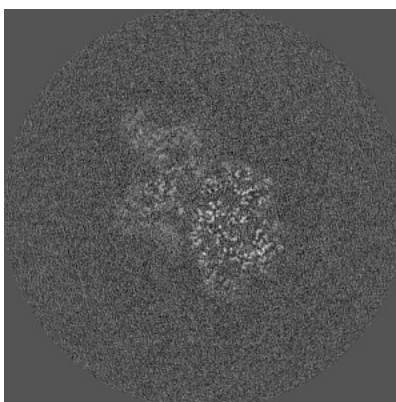


Z Index: 180

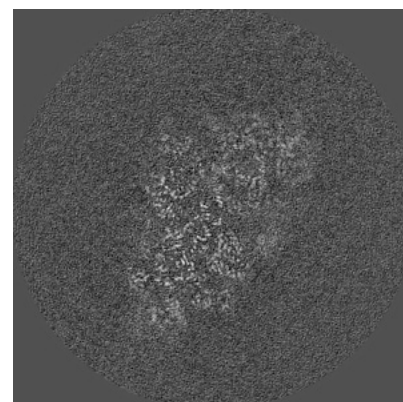
6.2.2 Raw map



X Index: 180



Y Index: 180

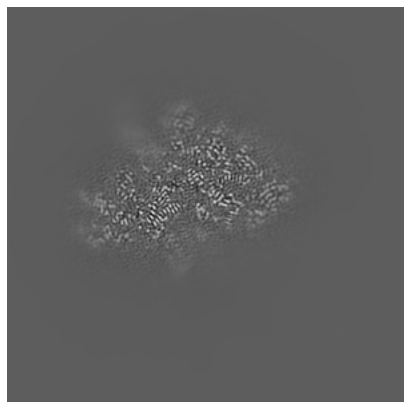


Z Index: 180

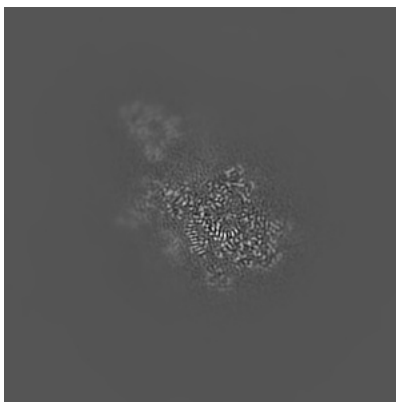
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

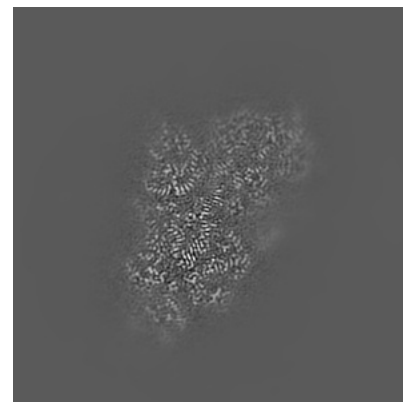
6.3.1 Primary map



X Index: 148

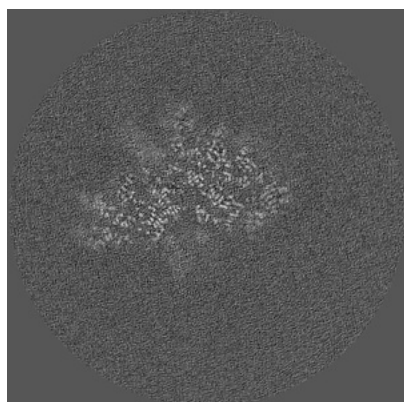


Y Index: 172

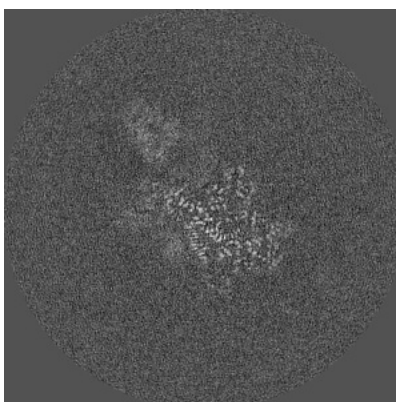


Z Index: 182

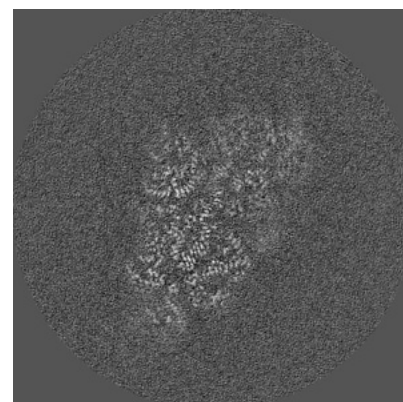
6.3.2 Raw map



X Index: 148



Y Index: 173



Z Index: 182

The images above show the largest variance slices of the map in three orthogonal directions.

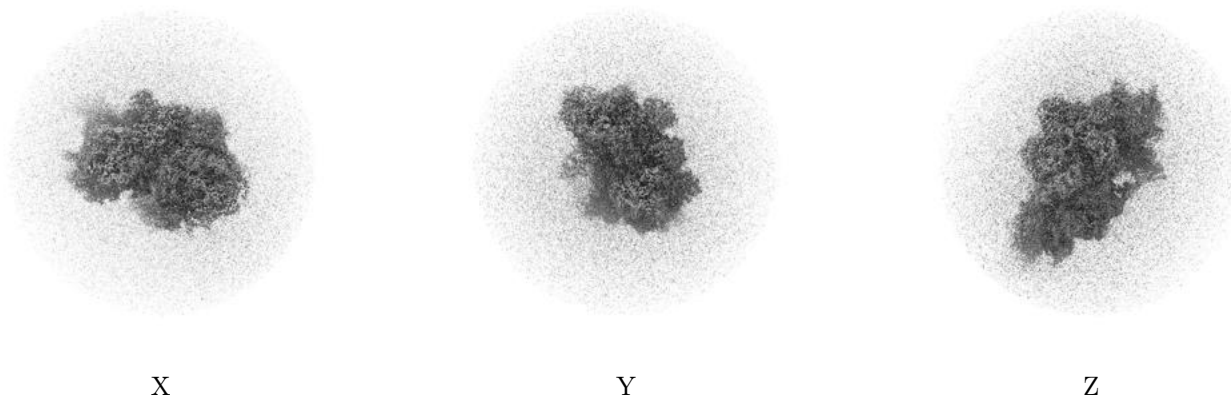
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

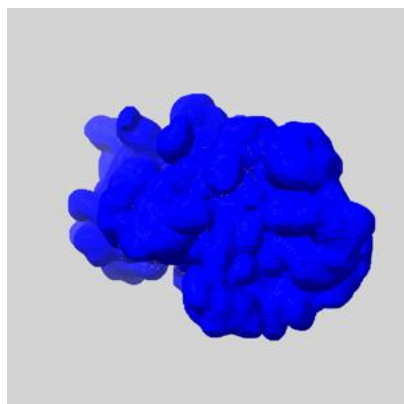
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

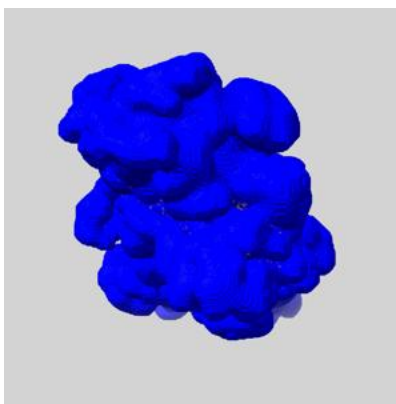
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

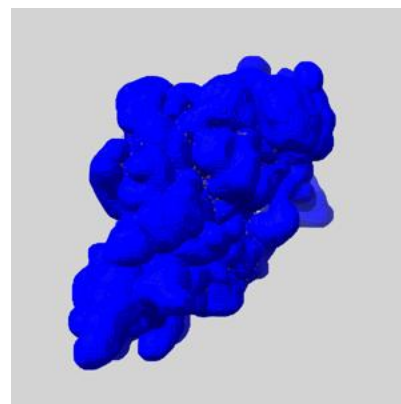
6.5.1 emd_11517_msk_1.map [i](#)



X



Y

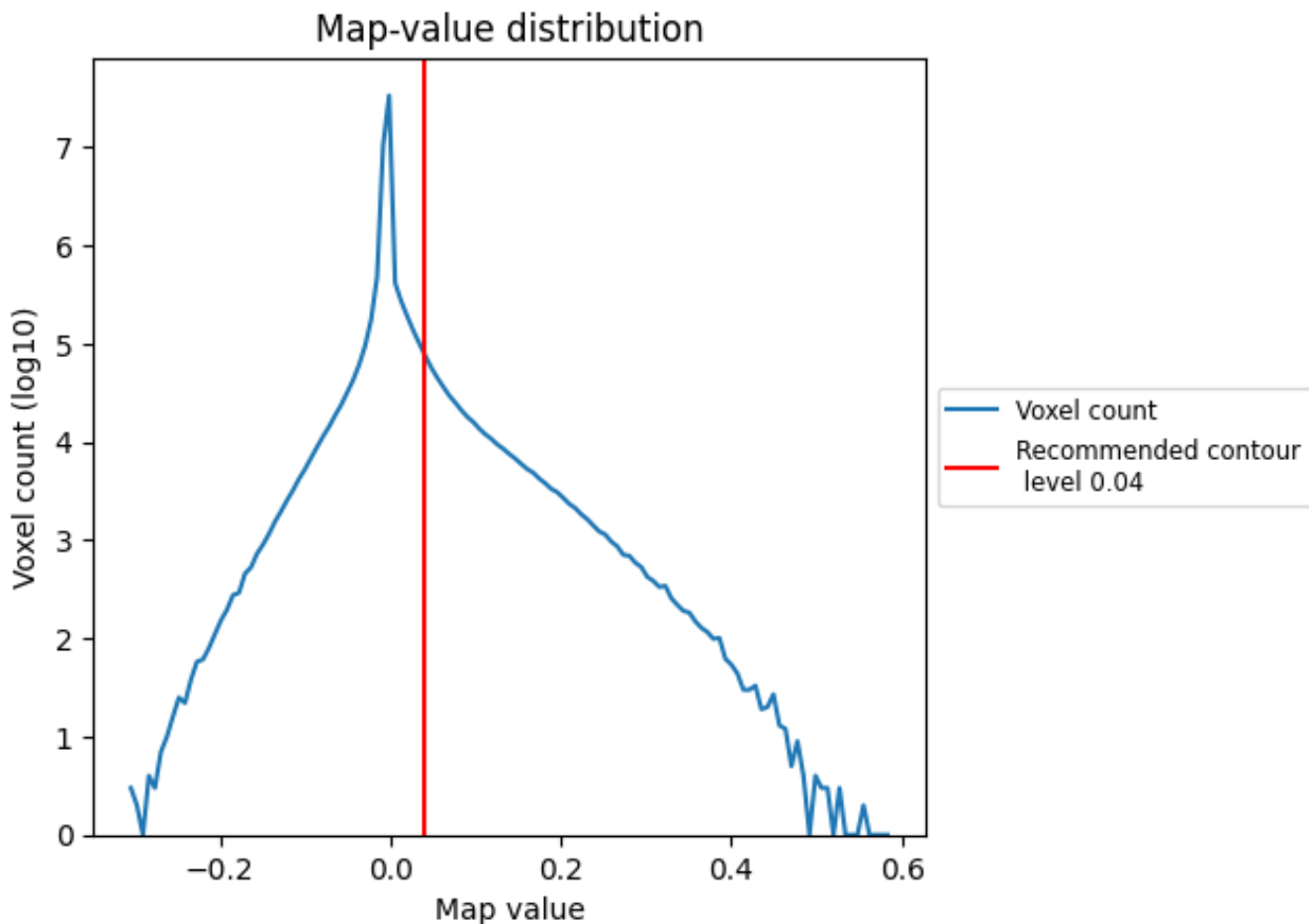


Z

7 Map analysis [i](#)

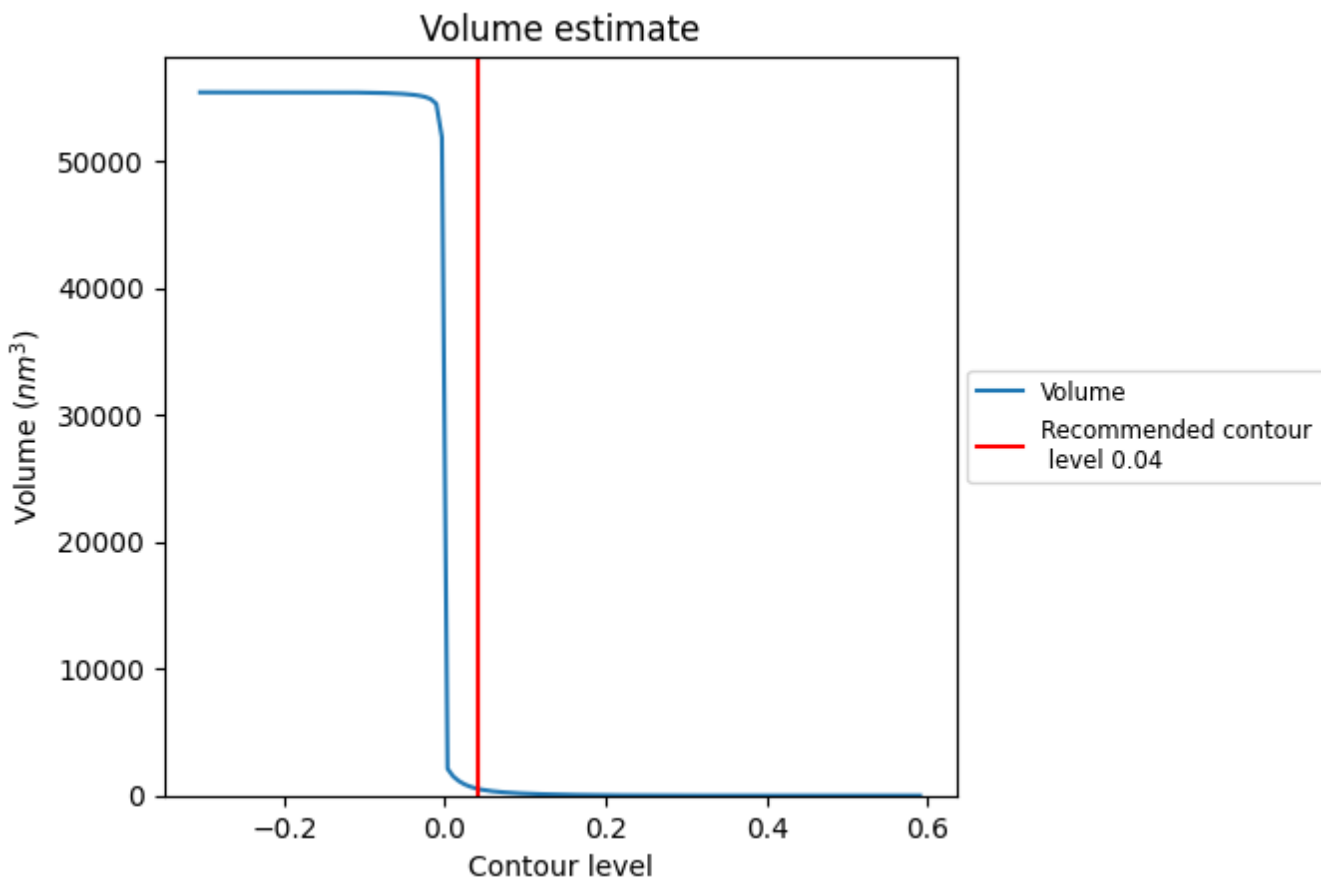
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

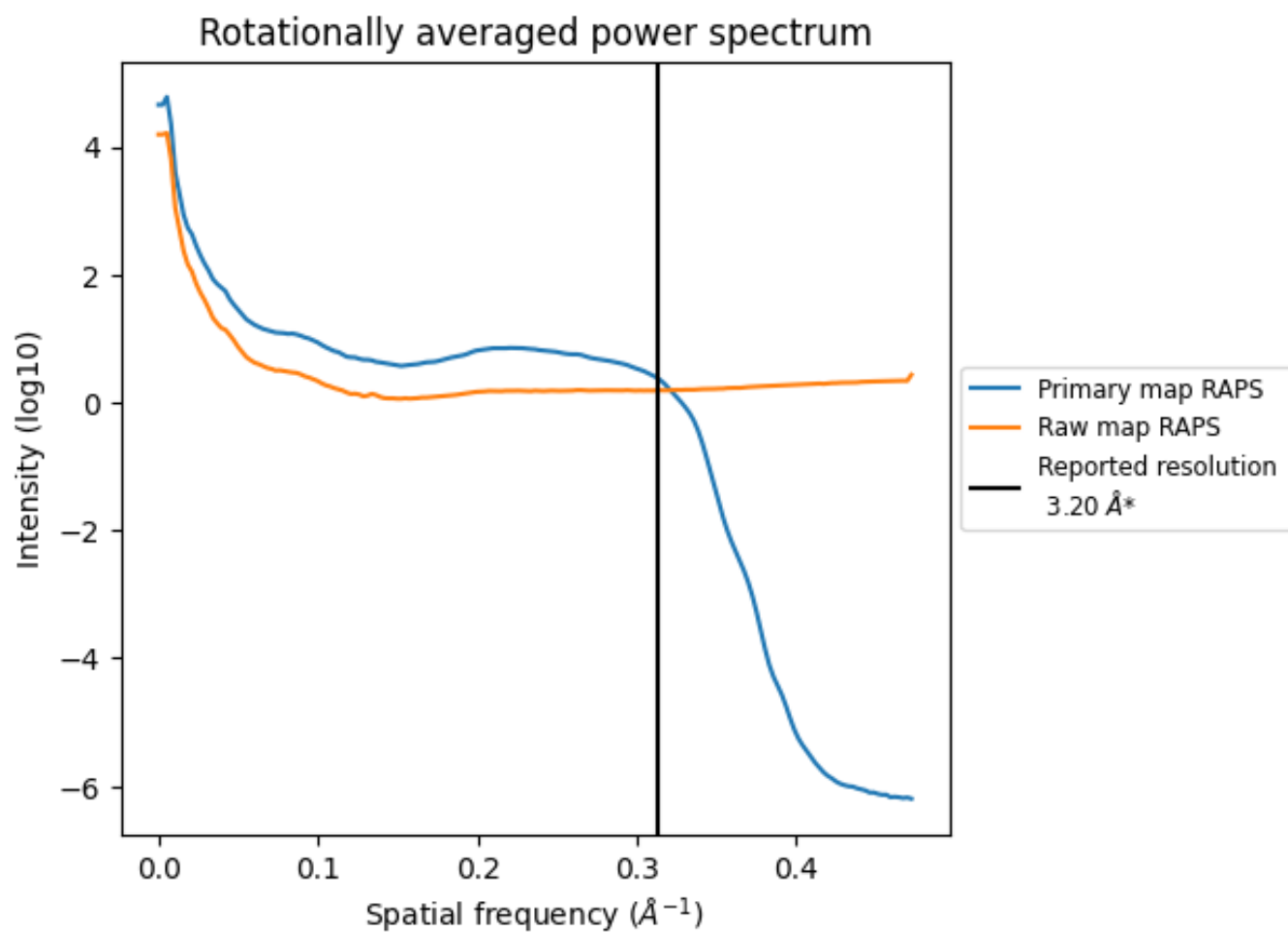
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm^3 ; this corresponds to an approximate mass of 494 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

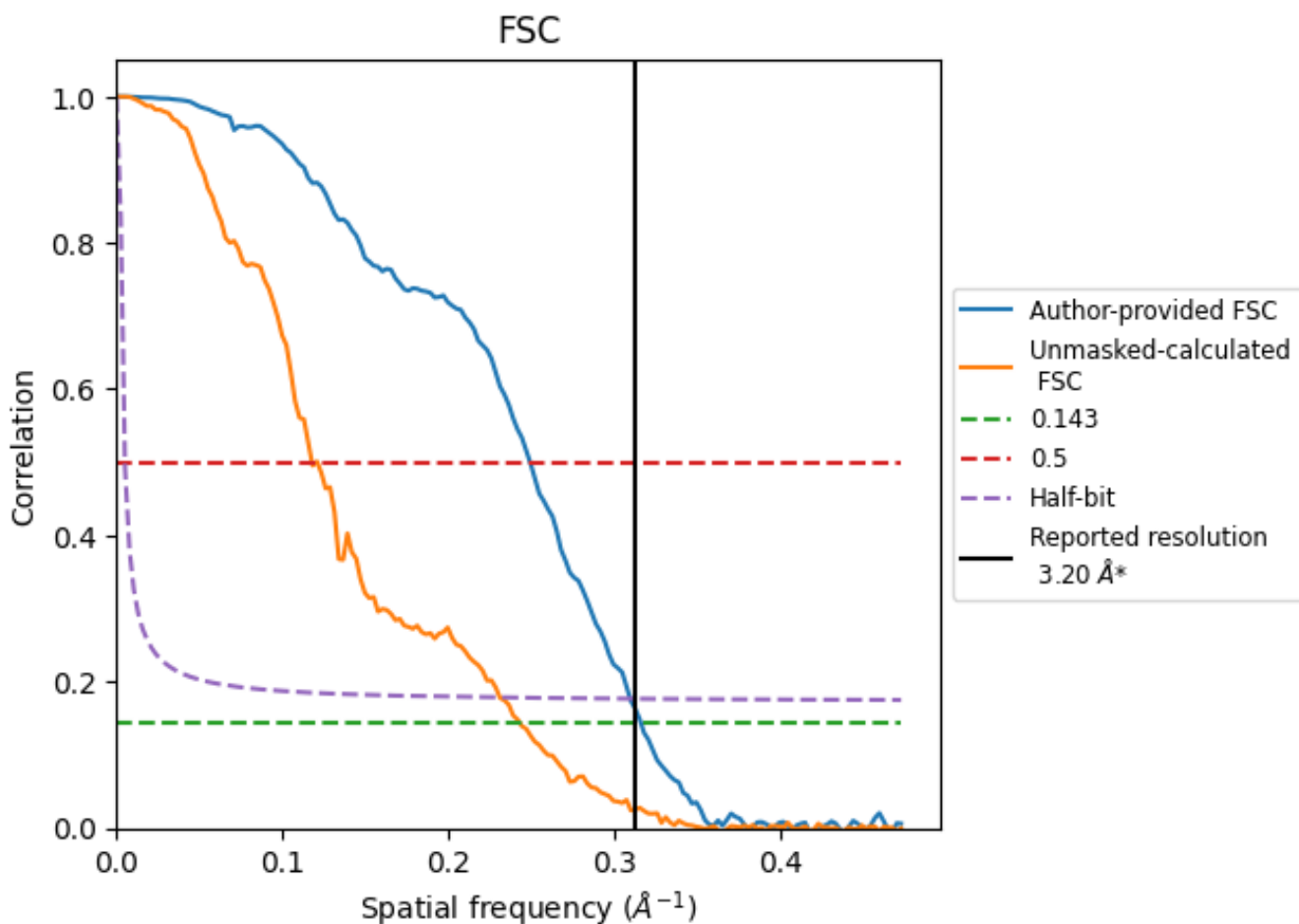


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

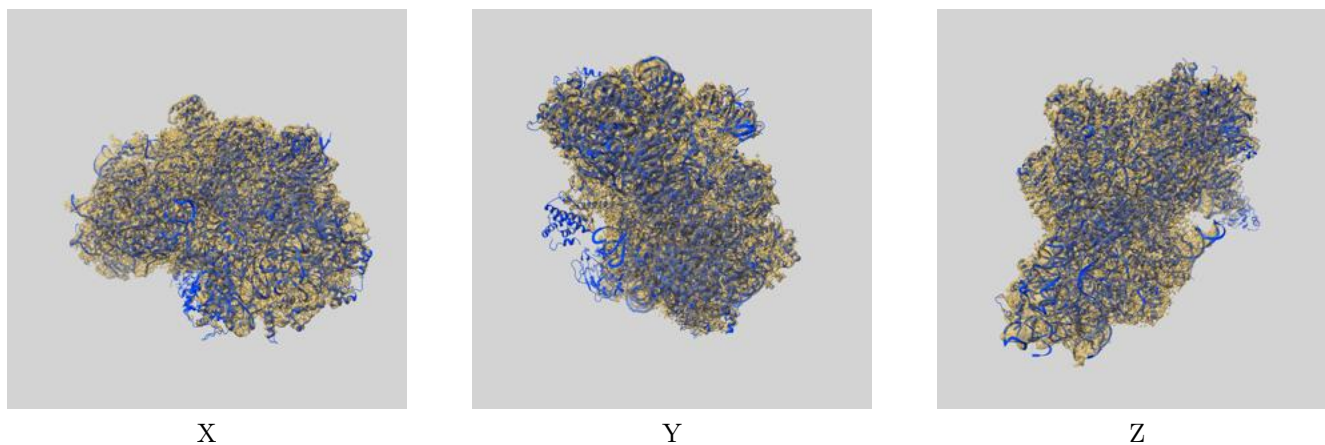
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	4.02	3.24
Unmasked-calculated*	4.12	8.50	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

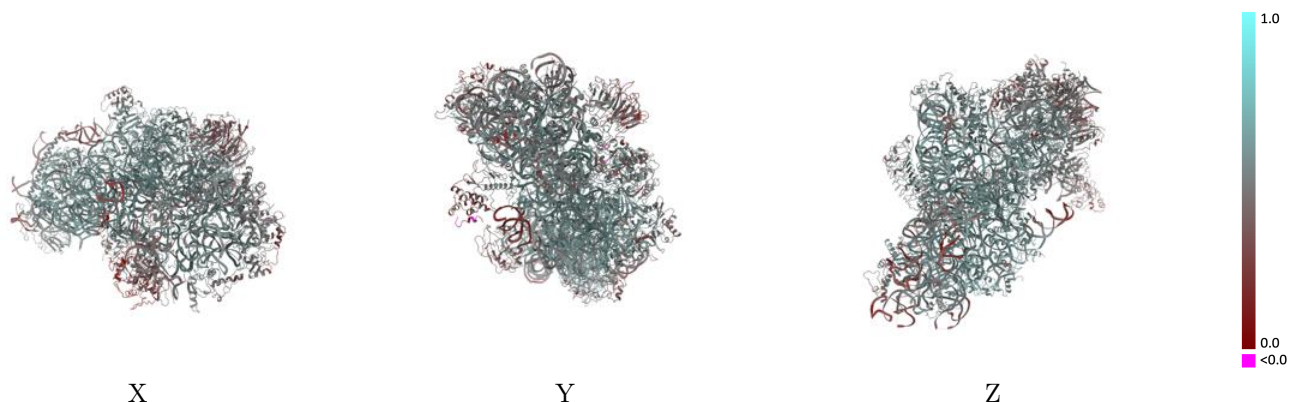
This section contains information regarding the fit between EMDB map EMD-11517 and PDB model 6ZXD. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



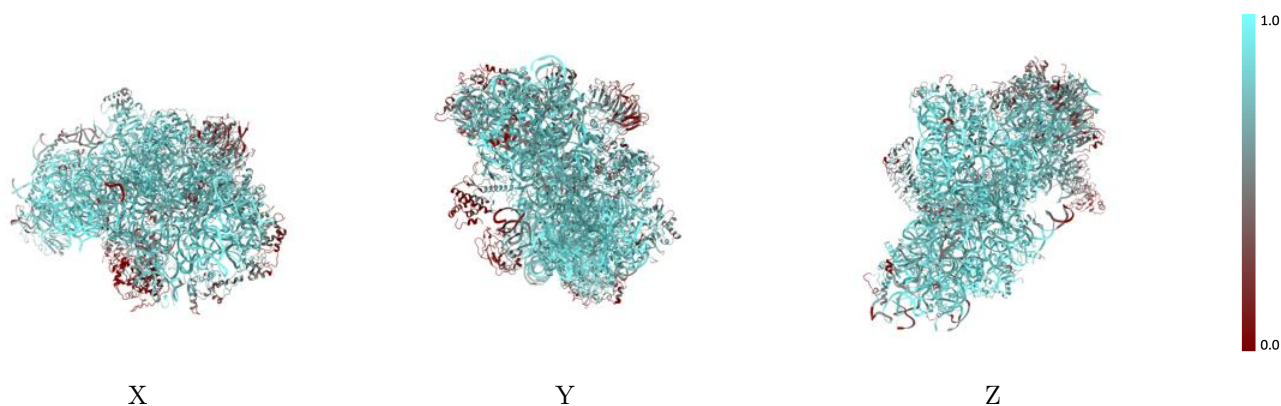
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



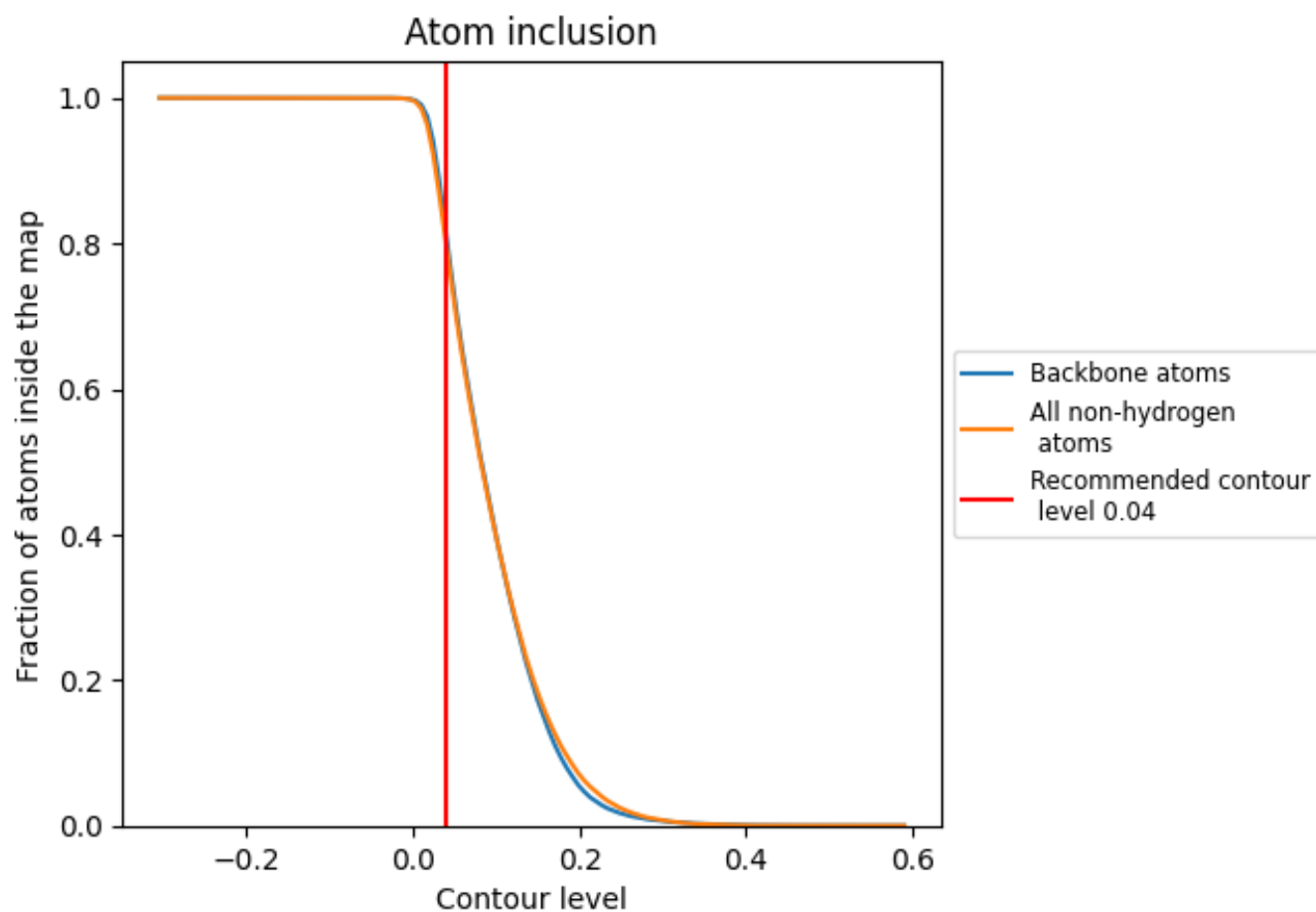
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary







The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7978	 0.5200
2	 0.8957	 0.5340
A	 0.8816	 0.5690
B	 0.8040	 0.5440
C	 0.9005	 0.5730
D	 0.6706	 0.4880
E	 0.8958	 0.5780
F	 0.6891	 0.4800
G	 0.7328	 0.5010
H	 0.7296	 0.4950
I	 0.8189	 0.5390
J	 0.8909	 0.5730
K	 0.6026	 0.4620
L	 0.8593	 0.5600
M	 0.1276	 0.3010
N	 0.8834	 0.5680
O	 0.7878	 0.5330
P	 0.6279	 0.4990
Q	 0.7735	 0.5140
R	 0.7401	 0.4950
S	 0.5478	 0.4560
T	 0.7106	 0.5130
U	 0.6138	 0.4920
V	 0.8871	 0.5670
W	 0.9446	 0.6010
X	 0.9244	 0.5940
Y	 0.8791	 0.5660
Z	 0.3422	 0.3910
b	 0.8503	 0.5560
c	 0.6204	 0.4690
d	 0.9161	 0.5750
e	 0.8889	 0.5810
f	 0.3873	 0.3320
g	 0.4597	 0.3990
k	 0.4691	 0.4620



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
x	 0.8700	 0.5610
y	 0.6911	 0.4770
z	 0.5079	 0.4350